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Highly-Resolved Numerical Simulation of the Turbulent Combustion Process in Experimental Burners

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This paper presents investigations of experimentally well-characterised turbulent flames with highly-resolved **L**arge **E**ddy **S**imulations (LES) and **D**irect **N**umerical **S**imulations (DNS). The combustion process is modelled with a flamelet-based approach, which assumes that the local turbulent flame structure can be described by an ensemble of wrinkled laminar flames. Good agreements between the simulation results and experimental measurement data is achieved. The governing equations are discretised with the **F**inite **V**olume **M**ethod (FVM). The numerical implementation is tailored for massively parallel simulations on a large number of grid cells. The computational efficiency benefits from the applied simple grid structure and the use of non-blocking **M**essage **P**assing **I**nterface (MPI) parallelisation.

1 Introduction

World energy consumption is mainly covered by burning fossil fuels such as natural gas, oil and coal but also sustainable fuels like biomass, biodiesel or biogas. As fossil fuels are limited and their combustion releases pollutants, their efficient usage is essential. To increase efficiency, a detailed understanding of the complex physical and chemical processes involved is required. Besides experiments, numerical analysis increasingly helps to understand combustion, exploiting the rapid increase of computational power in the past decades. As combustion in technical devices mostly occurs under turbulent conditions, the numerical investigation of the interplay between turbulent transport and chemical reactions is of high interest.

The governing equations for fluid flow and combustion are too complex to solve them directly for technical relevant combustors. To enable the simulation of such combustors, the governing equations are averaged in time or locally in space to reduce the computational costs. The averaging in time is termed **R**eynolds **A**veraged **N**avier **S**tokes (RANS) simulation, the filtering in space LES. These averaging operations lead to a loss of information on the smaller scales, which requires additional closure models. These closure models are developed based on theoretical considerations and on DNS of simpler geometries.

This work concentrates on highly resolved LES and DNS of more realistic geometries aiming to investigate and further develop existing combustion models. To avoid the excessive cost of the direct computation of a detailed chemical reaction mechanism, a tabulated chemistry approach is applied.

2 Numerical Approach

The investigations have been performed with the PsiPhi code. The code solves the implicitly filtered Navier Stokes equations for an incompressible flow of constant or variable

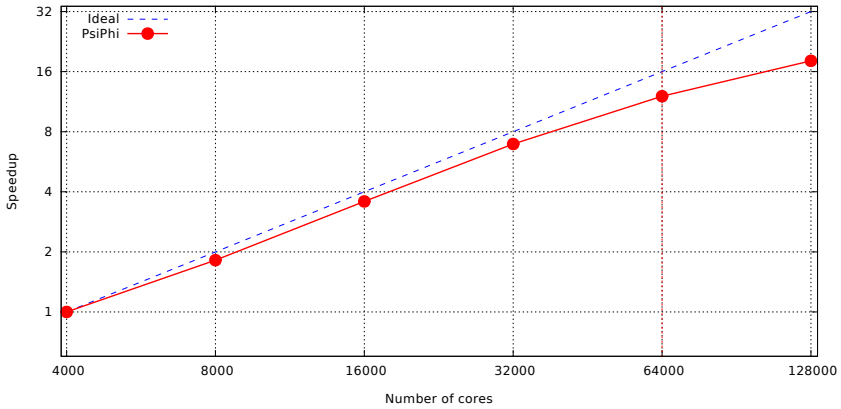

Figure 1. Strong scaling behaviour of PsiPhi on JUQUEEN. This test was performed with 1.6 Billion cells (i.e. 400,000 to 12,500 cells per core). The maximum number of cores used for the presented simulation results was 64,000.

density using a FVM. A Cartesian, equidistant grid is used, providing good numerical accuracy with isotropic filters, parallel efficiency and good vectorisation through avoiding slow, non-sequential memory access. Furthermore, this configuration allows to decompose the domain in blocks for maximum efficiency during communication between CPUs. Specific care has been devoted to efficient MPI parallelisation: PsiPhi is able to handle meshes with billions of cells, enabling highly resolved LES and DNS of laboratory scale configurations. To obtain a high parallel efficiency and performance of the code without the additional complexity of a hybrid approach, non-blocking MPI communication with overlayed computation is used. To assess the parallel efficiency, strong scaling tests have been performed on the JUQUEEN machine. The code performance has been tested on up to 128,000 cores, the respective results are shown in Fig. 1. The code scales well overall, for the maximum used number of 64,000 cores in the productive runs the parallel efficiency is around 70%.

PsiPhi ensures continuity by a pressure-correction scheme using a projection method. The transport equations are discretised with a 2nd-order central difference scheme in space and an explicit 3rd-order Runge-Kutta scheme in time.

The implemented chemical models enable the simulation of complex reacting flows. In the tabulated chemistry approach a small set of transport equations are solved for the conserved quantities, which describe the mixture composition and in addition the combustion progress. All thermochemical quantities are determined *a priori* and tabulated as a function of the control variables.

3 Quasi-DNS of a Bluff-Body Burner

The first presented case is a highly resolved simulation of an experimental bluff-body burner that has been investigated at the University of Cambridge and the Sandia National Labs[1,2]. The burner features a central bluff body that is surrounded by two co-annular

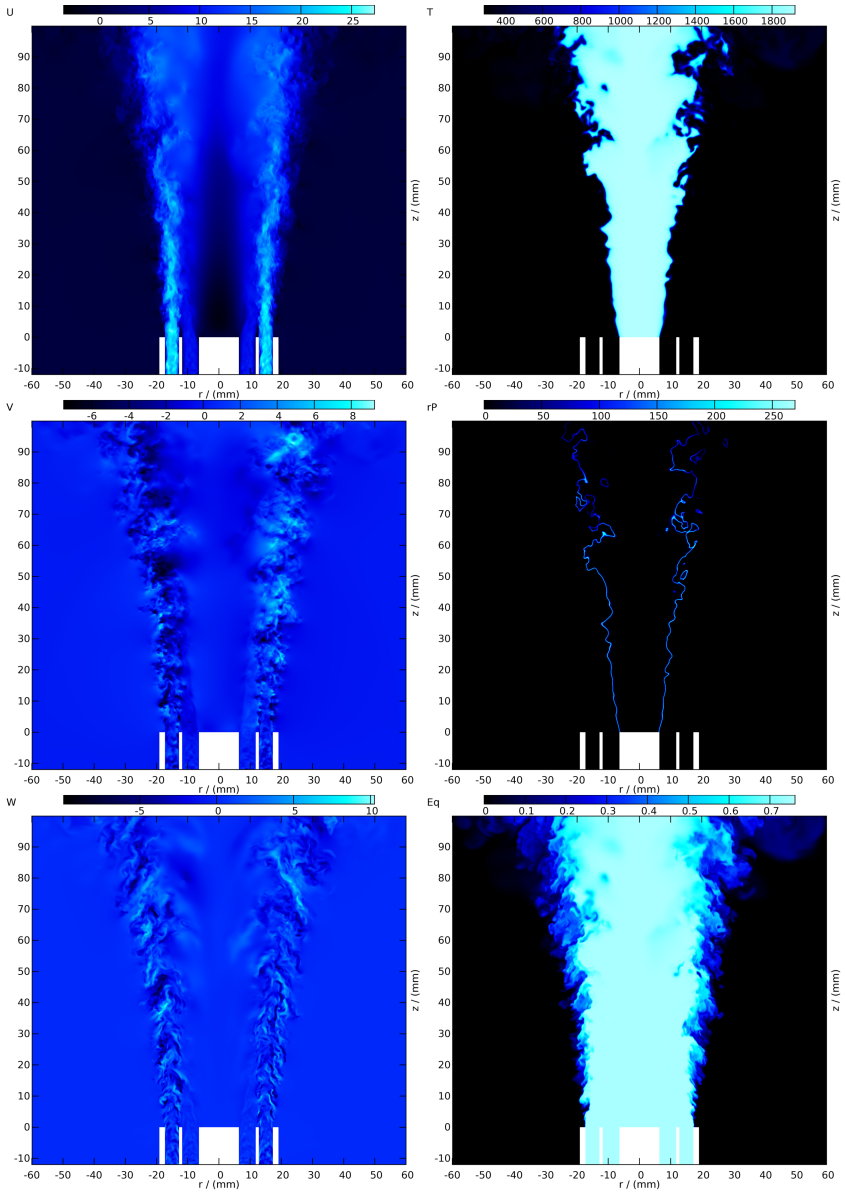

Figure 2. Contours of the velocity vector components (axial direction (U / (m/s)), radial direction (V (m/s)) and circumferential direction (W (m/s))), the temperature (T / (K)), the reaction source term (rP / ($\mathrm{kgm^{-3}s^{-1}}$)) and the equivalence ratio (Eq).

streams of lean premixed methane/air mixture at an equivalence ratio of 0.75. The whole burner is operated at ambient conditions and embedded in a co-flow of air. The grid resolution has been set to 100 μm, which is fine enough to resolve the turbulent flame struc-

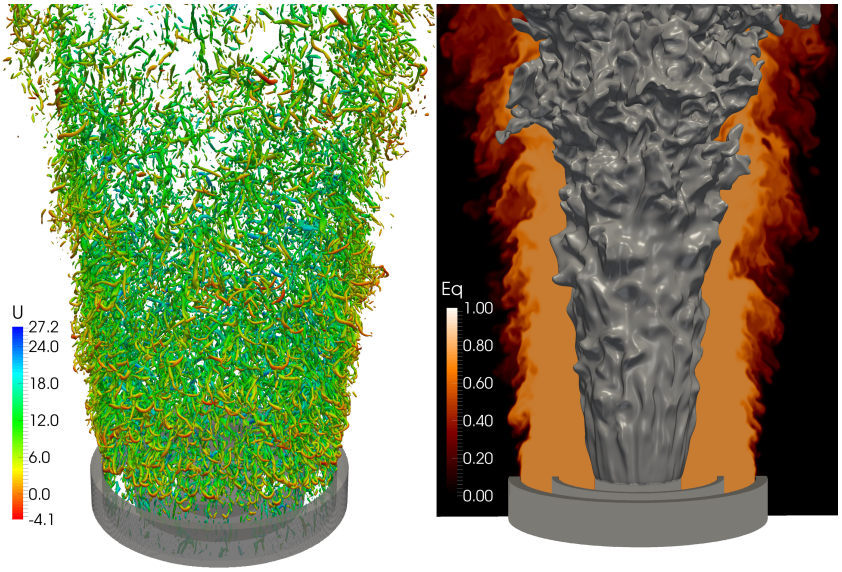

Figure 3. Left: Turbulent structures visualised by the Iso-q-criterion. The colouring corresponds to the axial velocity component (U / (m/s)). Right: Contours of equivalence ratio in the mid-section of the burner. The isosurface for 50% of reaction progress gives the flame location.

ture directly without any need for sub-filter modelling. This led to a total domain size of 1120x1200x1200=1.6 Billion cells. The combustion modelling is done with the **P**remixed **F**lamelet **G**enerated **M**anifolds (PFGM) tabulated chemistry approach. The work has been submitted to the Journal of Fluid Mechanics and is under review at the moment[3]. Fig. 2 shows contour plots in the burner mid-section for the velocity vector components (U, V, W), the temperature (T) and the reaction source term (rP). The recirculation zone in front of the bluff-body, which stabilises the flame, becomes clearly visible in the velocity plots. The velocity fluctuation levels vary in the inner and outer stream, and a large amount of the fluctuations is dissipated away in the flame region.

The equivalence ratio field is exposed to strong turbulent mixing due to the shear layer between the outer stream and the co-flow, the mixing layer is getting broader when moving downstream. In contrast, the flame thickness stays relatively constant, due to the balance between chemical reaction and diffusion. The reaction source term plot visualises the inner flame zone, it can be seen that the flame actually burns in two regimes: In the near burner region, the flame front is only mildly wrinkled and relatively laminar. In the region from approximately 35 mm downstream, the flame gets much more wrinkled due to the interaction with the turbulent fluctuations originating from the shear layer between the inner and outer stream. A statistical investigation and comparison to the Peters-Borghi diagram (not shown here) have confirmed this observation.

Visualisations of the resulting three-dimensional flow- and flame structures are presented in Fig. 3. The left plot shows the iso-q-criterion, which is computed from the second invariant of the velocity gradient tensor and gives a good impression of the rotating structures present in the flow-field. A broad range of vortex structure sizes occurs, which

develop and interact when proceeding downstream. The right plot shows an iso-surface of the inner flame zone and a contour plot of the equivalence ratio. Again, the two flame regimes as discussed for Fig. 2 become visible. The three-dimensional structure of the flame surface develops from surface-wave patterns near the burner exit to distinct three-dimensional pockets far downstream.

The first and second statistical moments (means and variances), obtained from the simulations are compared against the experimental data. Additional correlations, spectra and probability distributions were evaluated to gain a deeper understanding of the process and reference data for the subsequent development of models that can be used in less expensive LES and RANS simulations which are utilised in industry.

4 Large Eddy Simulation of Reactive Multiphase Flows

Liquid fuels, with their many advantages, are utilised in relevant technical applications such as IC-Engines, gas turbines or oil-fired boilers. These devices feature highly turbulent flow structures to increase the mixing of fuel and oxidiser and subsequently increase the overall efficiency. The LES method is a suitable technique for the simulation of premixed and non-premixed flames as outlined by e.g. Janicka and Sadiki[4], but it also showed the capability to describe reactive multiphase flows.

A well established test-case for the validation of numerical models is the Sydney piloted spray burner, which was investigated by Masri *et al.*[5] at the University of Sydney. The diluted ethanol spray flame is supported by a concentric premixed pilot flame, which provides the heat for the evaporation of the liquid droplets and subsequently to ignite the partially premixed main flame.

An Eulerian and Lagrangian approach is used to describe the gaseous and liquid phase respectively. The numerical particles, which interact with the gaseous phase, are treated as lists of arrays, where each rank (or core) has a separate list to improve the numerical efficiency. In the present study it was possible to use one numerical particle to describe one liquid droplet. This aforementioned treatment allows to have a better description of the particle distribution in the finite volumes. The PFGM approach combined with the **A**rtificial **T**hickened **F**lame method (PFGM/ATF) as described by e.g. Proch and Kempf[6] was adopted to fulfil the requirements to model the flame in the presence of a diluted spray, details can be found in the studies by Rittler *et al.*[7]. Source terms in the governing equations for the momentum, the mixture fraction and the reaction progress variable are required to account for the evaporating droplets. The unresolved velocity fluctuations are determined with Nicouds Sigma model[8], that yields the same accuracy as the Smagorinsky model with a dynamic procedure at much lower numerical costs.

As illustrated in Fig. 4 (a), the droplets evaporate due to the impact of the pilot flame and increase the mixture fraction further downstream, starting at z = 50 - 70 mm. Due to the higher slip velocity of the particles, that penetrate into the pilot stream from the jet stream, the evaporation is further amplified. The maximum mixture fraction is found at an axial location of z = 120 - 200 mm, downstream of this location the figures suggest that evaporation is completed. The spray flame has a lifted character at z = 50 - 70 mm, as outlined by the temperature and the OH mass fraction in Fig. 4 (b) and (c). Furthermore the OH mass fraction clearly indicates the flame wrinkling which results from the high turbulence level that increases mixing and the turbulent flame speed and reduces the flame

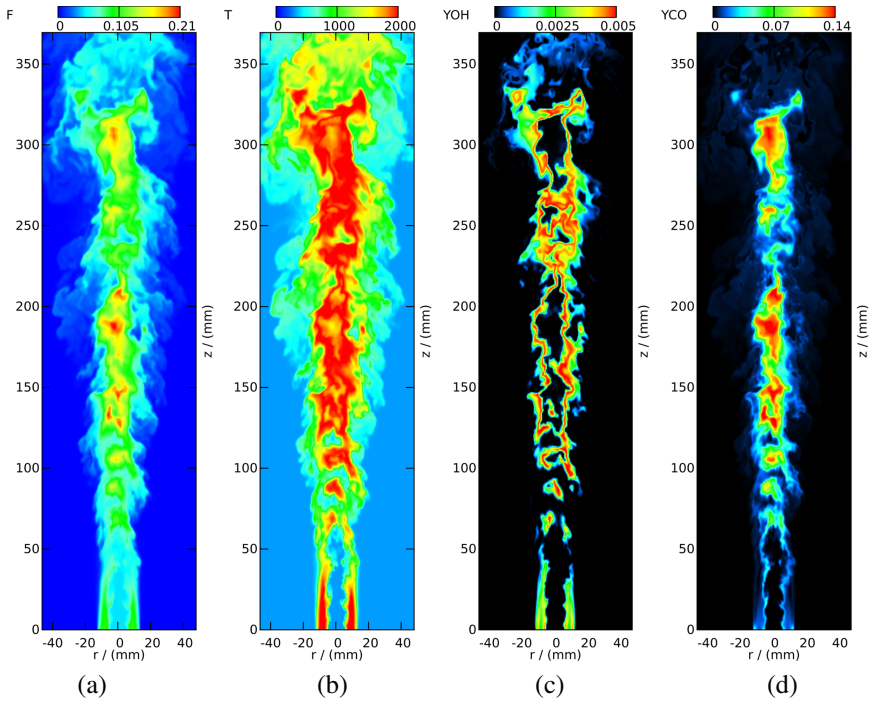

Figure 4. Contour plots of the simulation results for the (a) mixture fraction (F), (b) temperature (T / (K)), and the species mass fractions of (c) OH and (d) CO.

length and width. Besides this, OH indicates the flame front, which was found to be in good agreement with the experiments (not shown here). The applied model is also able to capture some toxic intermediate species like CO, as illustrated in Fig. 4 (d).

The modified PFGM/ATF approach is validated with the available data from the experiments - the first and second statistical moments for the particle properties and gas phase properties are in good agreement. Furthermore, a deeper understanding of the underlying processes in the spray flame could be obtained.

5 Massively Parallel Large Eddy Simulation of Pulverised Coal Combustion

Only since recently, computational power has become sufficient for the LES of realistic **P**ulverised **C**oal **C**ombustion (PCC) furnaces. However, as there are still open question regarding the modelling for the LES of PCC, validation against experimental measurements is indispensable. These measurements can only be obtained from laboratory up to semi-industrial experiments. Among these is the experiment by Weber *et al.*[9] conducted by the **I**nternational **F**lame **R**esearch **F**oundation (IFRF). We chose this experiment to validate our models since it offers a good compromise between comprehensive measurements and an environment comparable to large-scale furnaces found in power plants. In the future LES

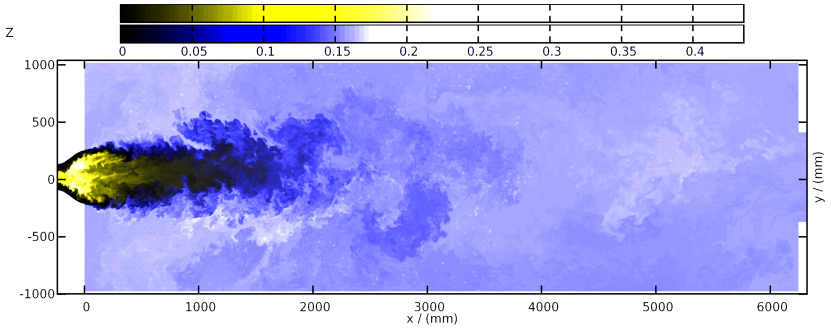

Figure 5. Instantaneous image of volatile gas mixture fraction (yellow scale) and char-off gas mixture fraction (blue scale) from the LES of the IFRF furnace.

of PCC promises to assist engineers and scientists in designing new and efficient furnaces and to obtain additional information that cannot be obtained by experiments.

The presented simulation relies on the non-premixed flamelet model to describe the gas phase. In the case of PCC, two mixture fractions have to be considered which represent: a) volatile gases released as the coal particles are heated up and b) the char-off gas that is released when oxygen diffuses into the porous coal structure during later stages of the coal combustion. Additional to the two mixture fractions, enthalpy and variance are required as parameters to describe the chemical state which leads to a four-dimensional pre-computed table that stores all the chemical information and is accessed during the computation.

An instantaneous image of the mixture fractions is shown in Fig. 5. It illustrates how volatile gases are released close to the inlet in the recirculation zone in the quarl region. Further downstream the burned volatile gases mix with combustion air promoting the slow char oxidation process through providing a hot mixture with oxygen excess.

Fig. 6 shows the CO_2 mass fraction. Intermediate CO_2 mass fractions can be found in the quarl region where mostly volatile gases burn. The CO_2 mass fraction first decreases further downstream as it is mixed with fresh combustion air. The highest CO_2 mass frac-

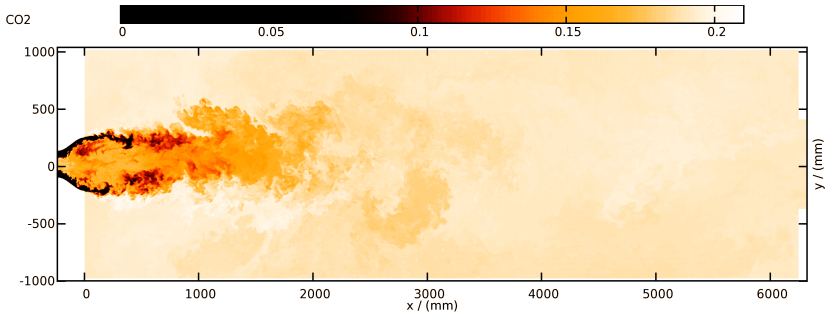

Figure 6. Instantaneous image of CO2 mass fraction from the LES of the IFRF furnace.

tions are found downstream where char oxidation takes place.

The furnace has been discretised with 1.7 B cells and 40 M particles. The cells have an edge length of 2.5 mm and one numerical particle represents 100 real coal particles. Coarser simulations and the validation of the flamelet model for the LES of realistic PCC are currently under review[10]. The data from the simulations is compared to the experiment by means of statistical moments of species concentrations, temperature and velocities. The data is further analysed with a focus on instantaneous particle and gas phase quantities to gain additional insight into the combustion process and to identify possible model improvements.

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